

Monte Carlo Computer Simulations of Irreversible Adsorption of Colloid Particle at Solid-Liquid Interface

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Colloid dispersion is a multi-phase system composed of a continuous medium in which one or more phases (particles) are dispersed. Colloid dispersions are very common in nature and industry. An important example is blood containing many bio-molecules and cells. Other common examples are milk, inks, paints, and wastewater. We focus on systems containing a liquid medium (usually water or electrolyte) and solid or liquid particles. By definition, colloid particle size is of the order of 1 – 1000 nm. Because of the very small particle size, colloid dispersions have an extremely large interfacial area between two phases: medium and colloidal particles, such that surface effects play much more important role than volume effects. This results in several characteristic properties of colloids. First, larger colloid particles scatter a light beam passing through them (Tyndall effect) due to reflection of the light by their surfaces. Next, because of their small mass, the particles undergo Brownian motion. Another interesting feature is spontaneous charging of colloid particles in a polar media like water. The origin of the charge may be adsorption of ions from the solution or dissociation of ionogenic groups at the particles' surfaces. Finally, due to their big surface area, colloids have a great adsorbing power.

Very often we are interested in collecting colloid particles at a solid surface. This may be either because we want to remove them from a suspension (e.g., wastewater filtration) or we need themselves for a further processing or application (e.g., enzymes immobilization). The phenomenon of collecting of colloid particles at a solid-liquid interface, called adsorption, has a great significance in many natural and practical processes such as membrane filtration, paper making, protein and cell separation, biofouling of membranes, organ

transplantation, and many other. Experimental observations of adsorbed colloid particles suggest that their adsorption is usually irreversible and localized. Again, it is a consequence of the large surface to volume ratio, which makes the electrostatic particle-interface attractive interaction much stronger than hydrodynamic forces.

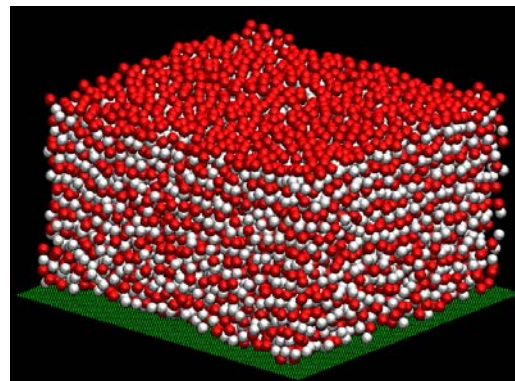


Fig.1. Adsorbed colloid particle multilayer composed of twenty layers. The first layer surface coverage is equal to 0.05. Red particles can be attached to white particles only and vice versa, except the particles of the first layer that are attached to the homogeneous adsorption surface represented by green dots.

Irreversible colloid adsorption can be modeled using a variety of approaches. Among them, the Monte Carlo random sequential adsorption (MC-RSA) approach seems to be the most suitable because of its simplicity and efficiency. The classical RSA model [1] considers a sequence of trials of monodisperse, spherical particle adsorption at a homogeneous interface, taking into account geometrical effects only. Since 1980s a number of extended RSA models have been developed that include the effects of particle shape [2], Brownian motion [3], external force [4], particle-particle and particle-interface electrostatic interaction [5], colloid-particle polydispersity [6], and surface heterogeneity [7]. Recently, the simulation algorithm has even been extended for multilayer adsorption simulations [8]. Fig.1 presents a colloid particle multilayer composed of twenty layers simulated using the extended RSA model. The results based on RSA simulations allow us to predict particle layer structure and the jamming coverage of particles. We can use the model to predict particle-adsorption kinetics as well, although, depending on the particle-transport mechanism, an appropriate analysis of real adsorption problems can require including a

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correction for bulk transport or the hydrodynamic scattering effect. Thus, RSA modeling can be a powerful tool in the study of irreversible adsorption of macromolecules, proteins, and colloid particles.

Figs.2 and 3 present the multilayer density distribution calculated with the extended RSA model for the multilayers composed of twenty layers with the first layer surface coverage equal to 0.01 and 0.30, respectively, under assumption that the particle density of the particles adsorbed in both even and odd layers is equal 1.0. We notice that at

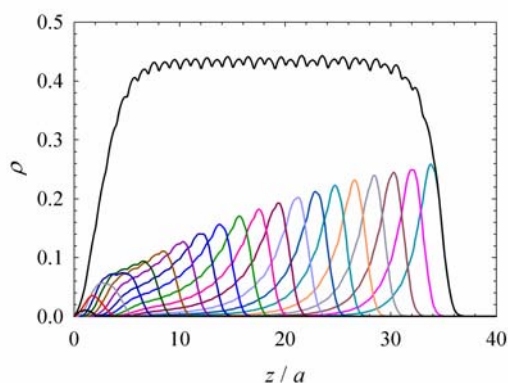


Fig.2. Multilayer density distribution calculated for the first layer surface coverage equal to 0.01. Color lines represent density distribution calculated for individual layers. The black line represents the total multilayer density distribution equal to the sum of the individual layer contributions.

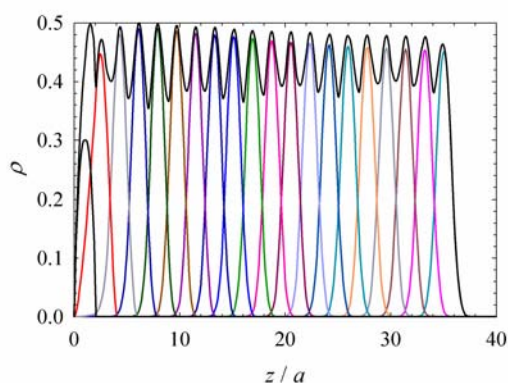


Fig.3. Same as Fig.2, but for the first layer surface coverage equal to 0.30.

the low coverage of the first layer the multilayer density distribution is relatively uniform while the high coverage of that layer results in large periodic changes of the multilayer density with the distance from the adsorption surface. These changes suggest that the structure of the multilayer simulated at the

high surface coverage of the first layer is more ordered than that simulated at the low surface coverage of the first layer, in agreement with intuition.

Acknowledgements

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